Abstract

The method of the electron in a network lattice allows to calculate the complete band structure of a complex crystal: one establishes explicitly a particular equation for each set of bands of the same type of symmetry. Besides the simplicity of the calculation we can point out as an advantage of such method the possibility of taking easily into account the influence of the atoms which are not merely the first neighbours, and the fact that the lattice potentials appear in the equations only as Dirac's functions.

Introduction:

The method for calculating the energy bands of the electron in crystals which we propose, is an extension of the "free electron network model" suggested by C.A. Coulson who has used it for "s" bands in metals.

With this generalization, which we shall call in the follow ing EN (electron netw.mod.), it becomes possible to calculate, rather easily the complete band structure of any crystal even if "complex", that is, with atoms of different chemical nature.

The simplicity of the mathematical framework lies essential ly in the fact that we consider, instead of the crystal, a geometrical model which allows to solve exactly Schrödinger's equation without using a variational method.

The lattice potential appears explicitly through Dirac's function $\lambda\,\delta(x)$ where λ characterizes the chemical nature of the atom. It appears also implicitly by a symplifying assumption on the form of the wave functions in the model which replaces the crystal.

In this model each atom is schematized by a polyhedron whose form and dimensions which are defined except for a homothetic of factor μ, are also characteristic of the chemical nature of the atom.

The potential $\lambda\,\delta(x)$ are localized on the vertices of the polyhedrons. A chemical band between two atoms is represented by a segment which connects the corresponding polyhedrons. In this way it is easy to take into account first, second neighbours etc...

To show clearly how the EN method works, we shall consider diamond type crystals and discuss briefly the case of complex crystals with particular regard to the II-IV compounds.

2. Description of the method

The fundamental principal of the EN, as stated in Technical Report n.5, is unchanged, we shall recall it here: "band structure in the FEN approximation is given by the variation against the wave vector $\vec{k}$, of the electron kinetic energy E on the branches of the network which are considered as lines of density current of the presence probability of electrons". However, since in the above stated report only first neighbours were considered, in the following we will show how the network should be modified with the addition of the second neighbours.

Fig. 1 shows that first neighbours are connected by segments which start from polyhedron, second neighbours are connected by segments which start from **different edges of the polyhedron.**

Fig. 2 shows the distribution of the wave function amplitude corresponding to the irreducible representation Δ'_2 .

Conclusion:

Owing to the fact that we are now considering 2nd neighbours as well, we have been compelled to rewrite all the equations and undergo a new set at calculations, which are now in process.

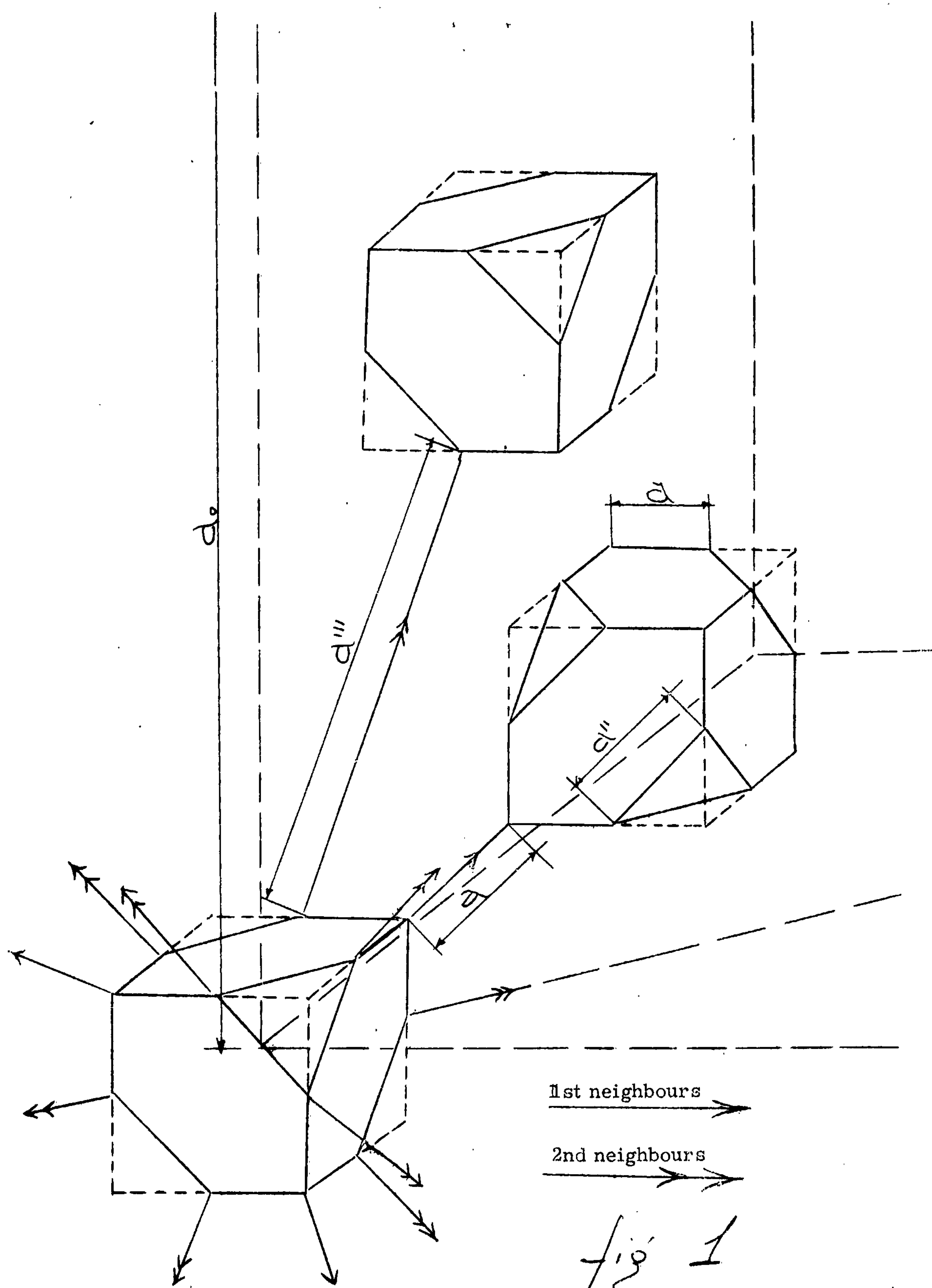
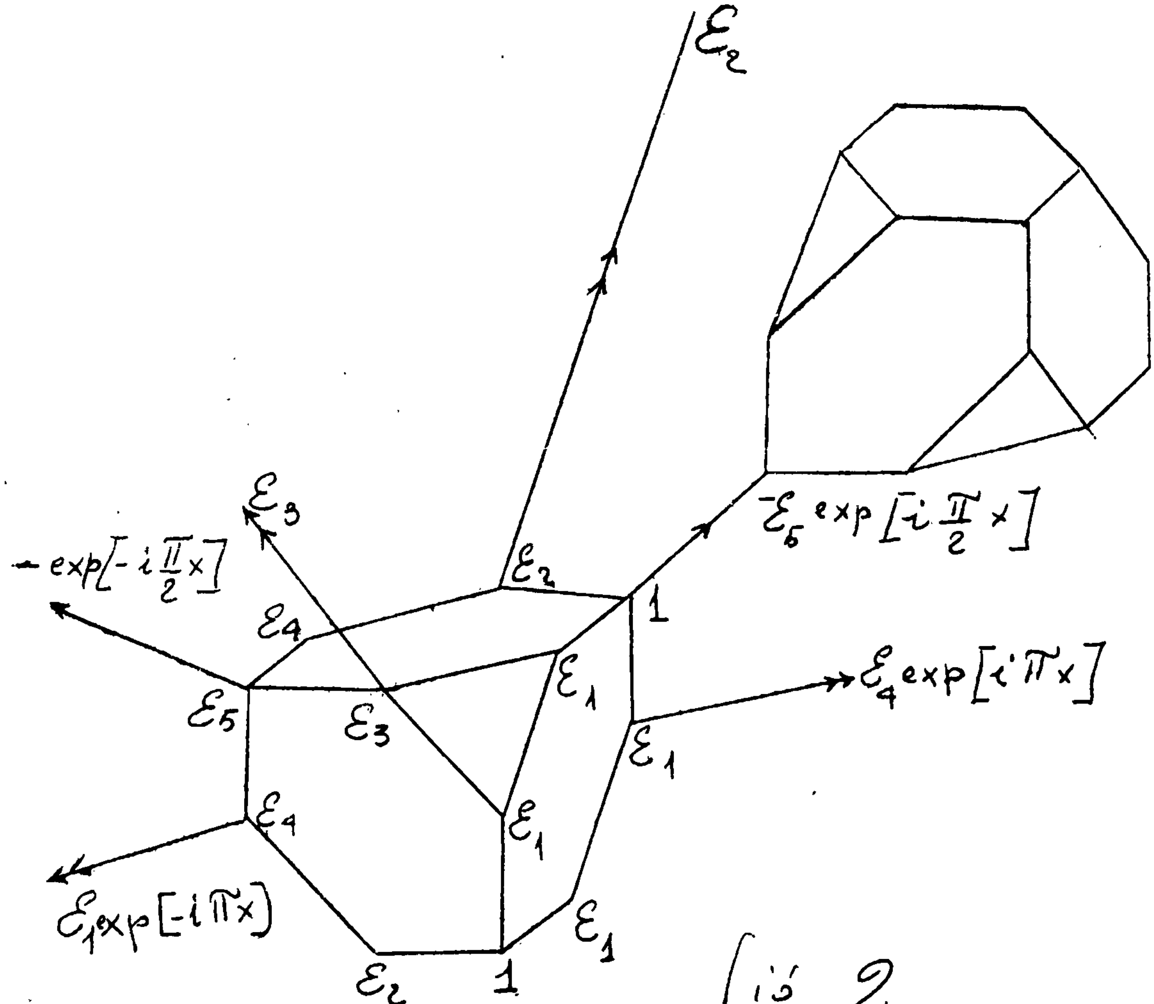


Fig 1



$\mathcal{E}_2$
$\mathcal{E}_3$
$-\exp[-i\frac{\pi}{2}x]$
$\mathcal{E}_2$
$-\mathcal{E}_5 \exp[i\frac{\pi}{2}x]$
$\mathcal{E}_4$
1
$\mathcal{E}_1$
$\mathcal{E}_4 \exp[i\pi x]$
$\mathcal{E}_5$
$\mathcal{E}_3$
$\mathcal{E}_1$
$\mathcal{E}_4$
$\mathcal{E}_1$
$\mathcal{E}_1 \exp[-i\pi x)$
$\mathcal{E}_1$
$\mathcal{E}_2$
1

fig 2